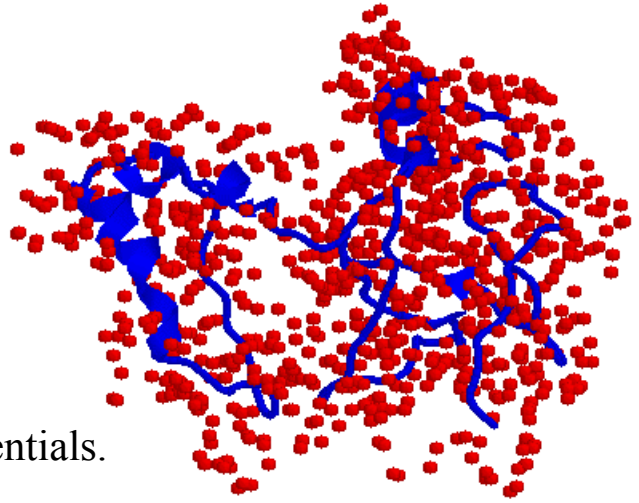
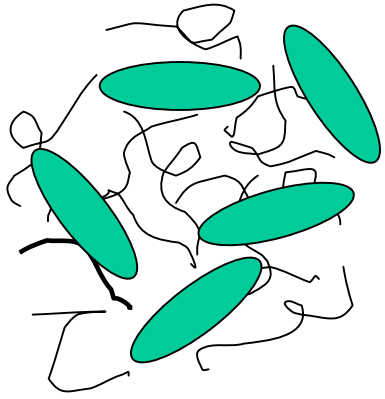
Coarse-Grained Simulation Methods for Complex Fluids: Venkat Ganesan: DMR 0204199



Our research focuses on developing simulation approaches for predicting the thermodynamics and dynamics of systems containing *many components, typically with disparate size, interactions and time scales*. Our recent work has focused on:

1. The effect of inert polymeric solvent molecules (denoted by red spheres on the first figure) on the phase behavior of protein solutions. This has been accomplished by the development of "implicit solvent" models to describe the interactions between the proteins by effective potentials. Simulations using such interactions were used to shed light on the thermodynamics of protein-polymer mixtures. These studies can prove important in understanding protein crystallization, aggregation behaviors which occur in contexts such as alzheimer's disease, cataract etc.



2. We have developed a new simulation tool to predict the rheology and properties of polymeric matrices containing a nanoscopic filler particles. This approach combines a molecular simulation approach for the particles with a coarse-grained method for polymers. We have sucessfully tested the method against a model system of a colloidal suspension in a simple fluid to glean new insights into the interplay between hydrodynamics and glass transitions. Our future work in this area is expected to shed light on practical strategies to manipulate the properties of polymer nanocomposites, a class of materials with unique strength, fire retardency properties.

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Education:

1 Graduate student (Ms. Surve) and 1 Postdoctoral associate (Dr. Pryamitsyn) are currently working on different aspects of this project. The inclusion of a Ms. Surve into graduate research helps in promoting theoretical materials science research among women, a traditionally underrepresented group in this field. As a part of their education, both of them are attending and presenting their researches at the American Institute of Chemical Engineers Annual Meetings. Dr. Pryamitsyn attended and presented his research at the Gordon Research Conference on Polymer Physics.

Outreach:

We have become involved with the Office of Equal Opportunity in Engineering (a program aimed at increasing the minority representation in Engineering) at Austin to explore if some of our simulation modules can be used in their outreach programs. Further, through this interaction, we have recruited a minority student Rick Ramos (a hispanic) who is planning on working on the self-assembly of rod-coil polymers.

We have also become involved with the RPI's initiative Virtual Polymer Laboratory(http://block.chem.rpi.edu/html/E_Outreach/) , to incorporate some simple simulation modules to demonstrate molecular concepts of polymer physics to high school students.